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TITLE: FUNDAMENTAL UNDERSTANDING OF MATTER: AN ENGINEERING VIEWPOINT

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FUNDAMENTAL UNDERSTANDING OF MATTER: AN ENGINEERING VIEWPOINT

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ABSTRACT

Fundamental understanding of matter is a continuous process that should produce physical data for use by engineers and scientists in their work. Lack of fundamental property data in any engineering endeavor cannot be mitigated by theoretical work that is not confirmed by physical experiments.

An engineering viewpoint will be presented to justify the need for understanding of matter. Examples will be given in the energy engineering field to outline the importance of our further understanding of material and fluid properties and behavior. Cases will be cited to show the effects of various data bases in energy, mass, and momentum transfer. The status of fundamental data sources will be discussed in terms of data centers, new areas of engineering, and the progress in measurement techniques. Conclusions and recommendations will be outlined to improve the current situation faced by engineers in carrying out their work.

1. INTRODUCTION

Good theories and elegant computer models can come crashing down about our heads if there are no valid properties of materials to use with them. This apparently obvious statement has been proven by many of us when we find work progress halted, incorrect decisions made, or useless paper studies published because the properties of materials were misapplied, ignored, or simply not available.

Early training of an engineer rarely includes an appreciation of continuous need for progress in fundamental understanding of matter. An exposure to limited sources for physical data paints a simplified picture of reality. Only when the engineer is confronted with a conflicting variety of sources, or a lack of sources, for information that reality becomes problematic.

Consider, for a moment, the thermal conductivity of copper at 400 K. Figure 1 includes all the pertinent thermal conductivity data in the literature.[1] It is impossible to pick a value unless a recommendation is given for a choice between 30 and 43 W/m.K. The recommended value by the Center for Information and Numerical Data Analysis and Synthesis (CINDAS) is 39.2 W/m.K. The deviation from the real value cannot be mitigated by fancy thermal analysis. How about the thermal conductivity of lithium oxide (Li_2O)? Suppose the heat transfer study of a fusion blanket required this.[2] Lithium

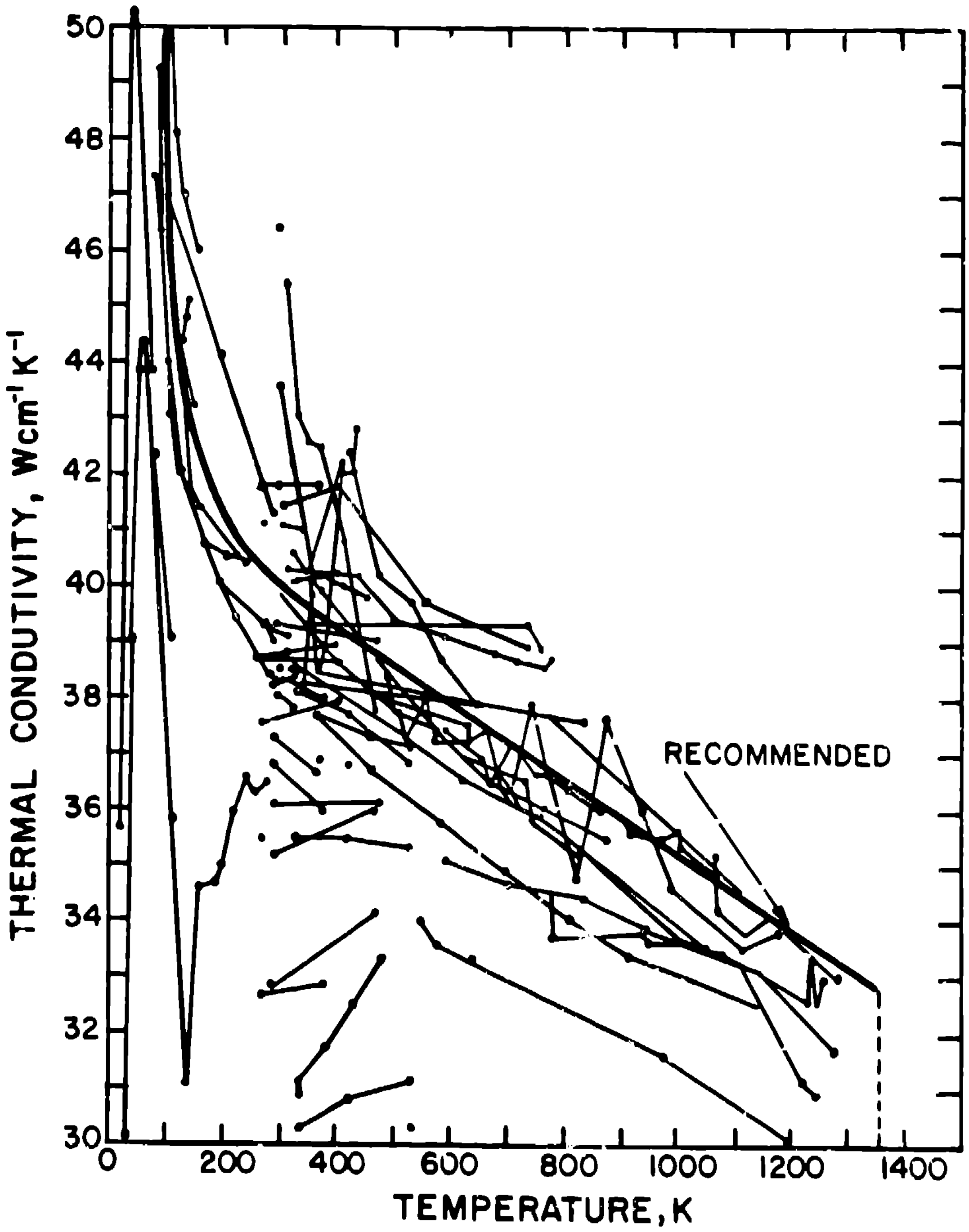

Fig. 1. Thermal Conductivity Data for Copper[1]

oxide in pellet form is considered a potential blanket material for tritium breeding (see Fig. 2). However, nobody has reported any data for the thermal conductivity of Li_2O. We have no choice but to estimate a value because of the time and budget constraints of a small study.

We will present an engineering viewpoint to justify the need for understanding of matter. Examples in the alternative energy sources field will demonstrate the importance of greater knowledge of properties of matter. Fundamental data sources will be discussed and recommendations will be given for improved property data so that better engineering of components and systems is possible.

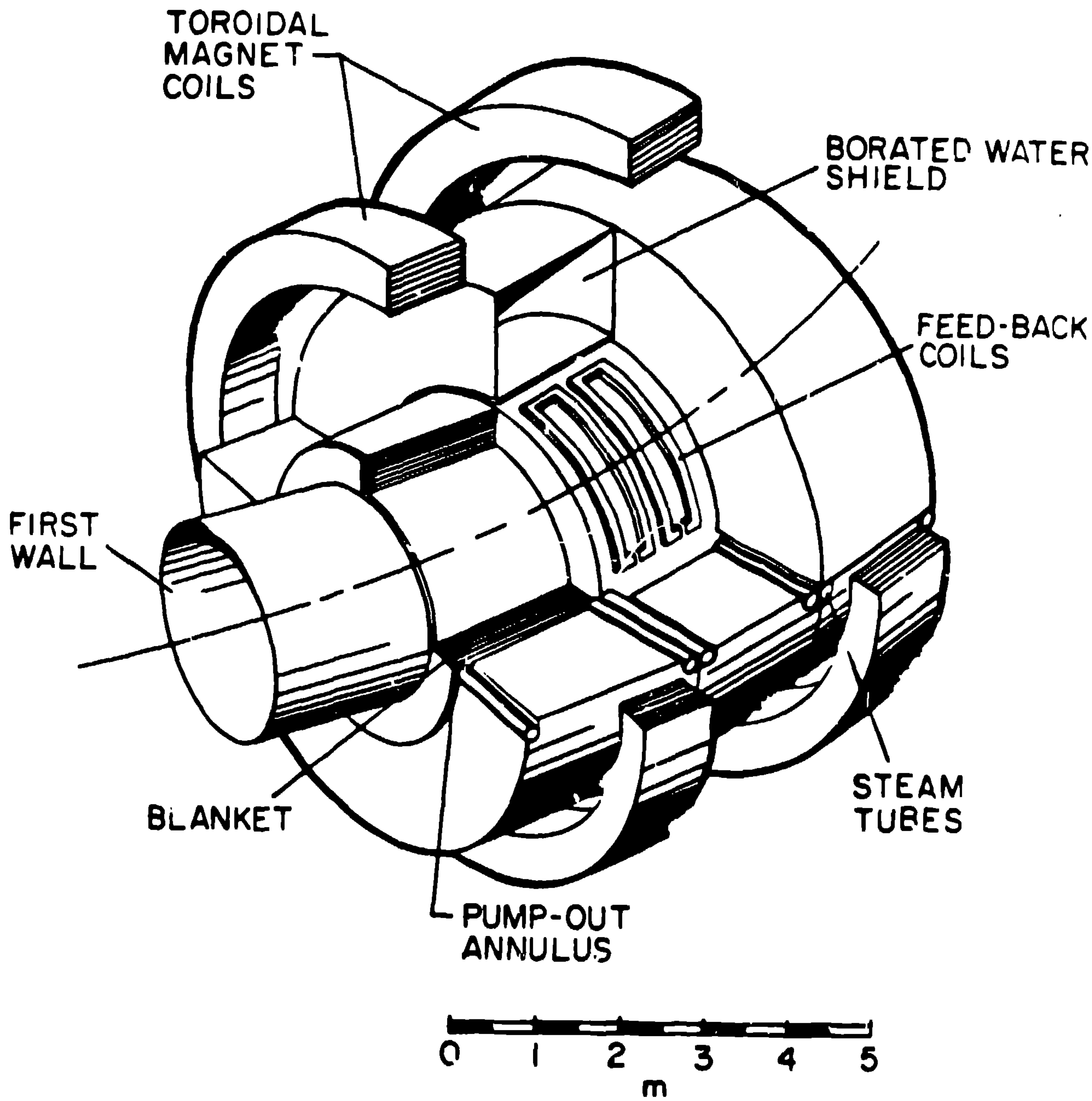

Fig. 2. Isometric view of four 2-m-long RFPR reactor modules, including the copper first wall, Li_2O blanket and associated high-pressure steam tubes, feedback coils, water shield, and toroidal coil.[2]

2. STATE OF AFFAIRS IN ENERGY FIELD

The general assurance of quality in any engineered component or system requires accurate performance analysis that uses precise properties of matter involved and proper modeling of the governing physical/chemical phenomena. Nowadays it is recognized that a modeling effort and/or testing program should be implemented as needed to support design engineering. What is not always supported is a continuous need for a better understanding of all the physical matter in our world. It is not always recognized that eloquent theories (or experiments) can be no more accurate than the properties used in these theories (or in experimental analyses).[3] We need systematic studies and analyses of accurate property information as science and technology progress.

In the field of alternative energy sources, the need for a better and greater knowledge of properties of matter is especially acute because of the following circumstances.

2.1. New Applications

Old, familiar materials are being used in new applications. The first example is the use of concrete in a vacuum environment. Recently, we considered concrete for a potting material for the focusing quadrapole electromagnets in a linear accelerator line.[4] This work was done in support of the Fusion Materials Irradiation Test Facility. A search of the vacuum, concrete, and reactor literature did not produce relevant data for concrete outgassing in vacuum.

Another example is the use of copper as a first-wall material in a fusion reactor concept.[2] A 20-mm-thick copper first wall was needed as a conducting shell to provide short-term eddy currents for stabilization of gross MHD modes on a ~ 0.1-s time scale (see Fig. 2). Our knowledge of copper in the operational environment of this reactor concept is severely limited.

2.2. New Materials

New materials are being developed, along with new processes and techniques, for improving their capabilities. For example, GRAPHNOL is a bulk graphite product developed for special-duty service in ballistic and other types of military missiles.[5] This new product is superior to conventional graphites because of a 50% improvement in resistance to thermal shock, almost 100% improvement in fracture strain, a 10% increase in thermal conductivity, a better flexure strength, and a cost which is a fraction of that for most carbon-carbon fiber composite materials. Potential applications include erosion resistant limiters, beam stops and first walls for fusion devices or reactors, and special radiation-resistant nuclear grades for use as moderator and reflector in high-temperature gas-cooled reactors.

2.3. Efficiency and Reliability

The need for greater energy efficiency leads to the use of materials and fluids very close to their ultimate performance limits. The melting point of solids or the boiling point of liquids are approached by design or, in practice, under off-normal conditions.

2.4. Improved Instrumentation/Methods

Improvements in instrumentation and experimental methods mean that more accurate and comprehensive measurements of the properties of materials/fluids can be made. New equipment, techniques, and models are allowing physical scientists to gather more precise data, thus leading to better theories on a wide range of physical/chemical systems.[6] For example, the National Bureau of Standards (NBS) has developed a system to test the properties of materials while they are heated to temperatures up to 3500°C (Ref. 7). The technique provides more than 1200 measurements in less than a second as the sample is heated with an electric current to the 1200–3500°C range. The measurements provide data on temperature and absorbed power, which are used to calculate properties such as heat capacity, electrical resistance, and thermal emittance. The measurement system will help our understanding of properties and behavior of metals and alloys, and improve prospects for using metals and alloys at elevated temperatures.

Steady improvement is possible in understanding physical/chemical events at their fundamental levels. Lasers are now being used to give higher resolution, faster, and easier-to-process spectroscopic information than is possible with other light sources.[6] Thus, previously unobtainable information on chemical products of combustion reactions may now be obtained with laser instrumentation. In addition, better computers and better software for them are revolutionizing the experimental physics and chemistry fields. The availability of inexpensive computers, analytical instrumentation suitable for on-line remote control, and interactive graphic terminals are accelerating progress in scientific and R&D efforts.[8] In the future, more analytical instrumentation will be self-calibrating and on-line with real-time graphic systems. The experiments will be controlled with self-adaptive algorithms to reduce the time required to understand complex systems. Also, interactive models and experimentation systems will be used for continuous data reduction with the capability to evaluate the progress of an experiment.

Figure 3 demonstrates an application of a computer-based digital enhancement and analysis method that was developed at the Los Alamos National Laboratory for transmission electron microscopy micrographs.[9] This method can be used to analyze overlapping images and void size, number, and location. The method is based on transformation of the photographic data of the TEM micrographs into a digital form that can be used by a computer. Figure 3a and 3b are TEM micrographs of high-purity (99.9999%) Al irradiated with 800-MeV protons at 50°C to a dose of 0.05 displacements per atom. These micrographs were selected because the large contrast range made them difficult to analyze using standard techniques. As shown in Fig. 3c and 3d, the difficulty in printing and analyzing the high contrast data has been eliminated, and defects are more identifiable.

2.5. Information Explosion

The "information explosion" makes it more difficult to locate relevant data. More often than not, a search for data stops after one or two results are found or after the searcher decides he has spent enough time looking. Figure 4 shows the trend over the years in getting improved data for the thermal conductivity of liquid toluene at 20°C to show that it pays to search.[11]

2.6. New Environments

New energy technologies require materials that stand up to increasingly hostile environments such as the blades for high-temperature gas turbines driven by combustion products from fluidized-bed coal furnaces. Also, many measurement discrepancies can occur when an apparatus calibration based

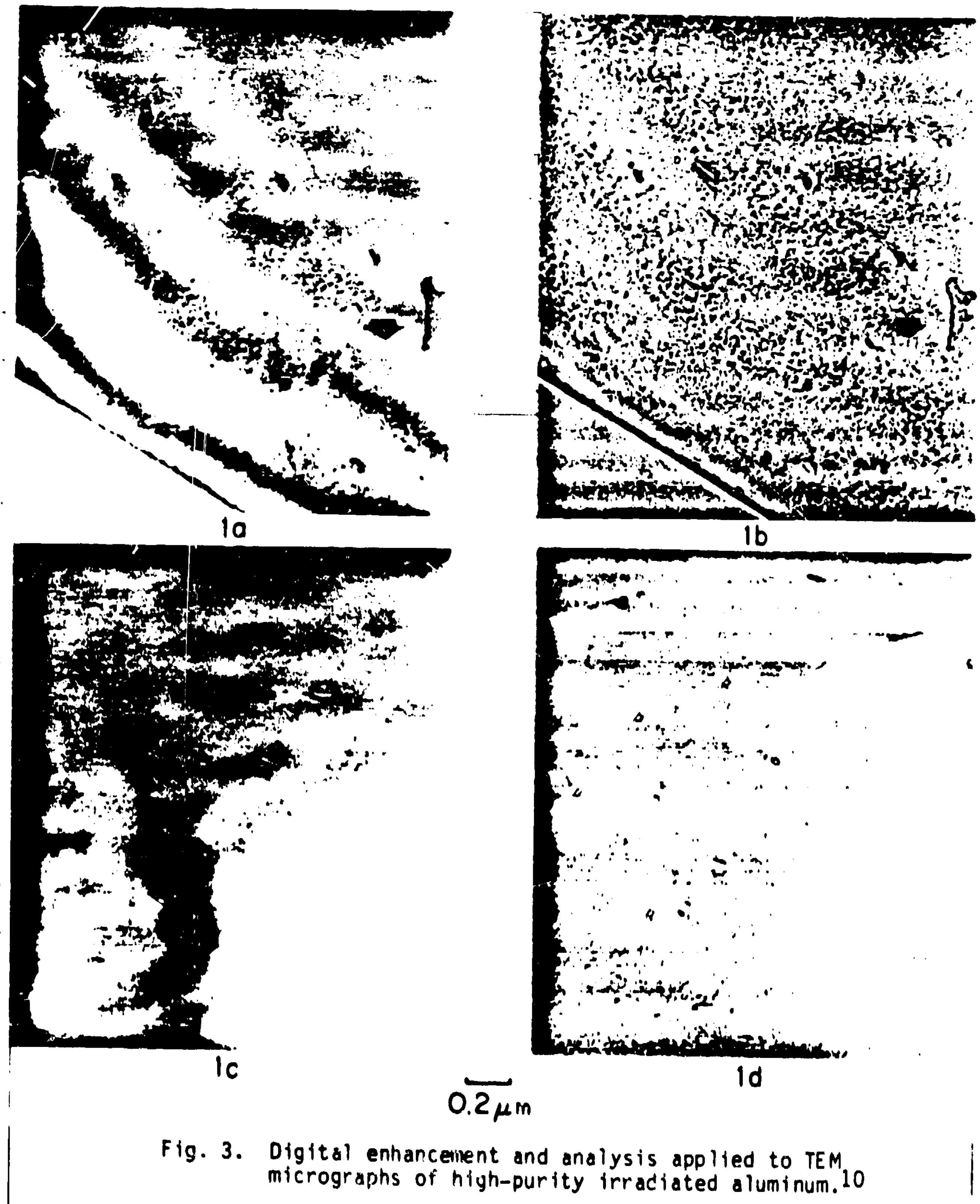

Fig. 3. Digital enhancement and analysis applied to TEM micrographs of high-purity irradiated aluminum.[10]

on the current NBS thermal reference standard is extended to these environments, which are different than those for which the standard was developed.[12]

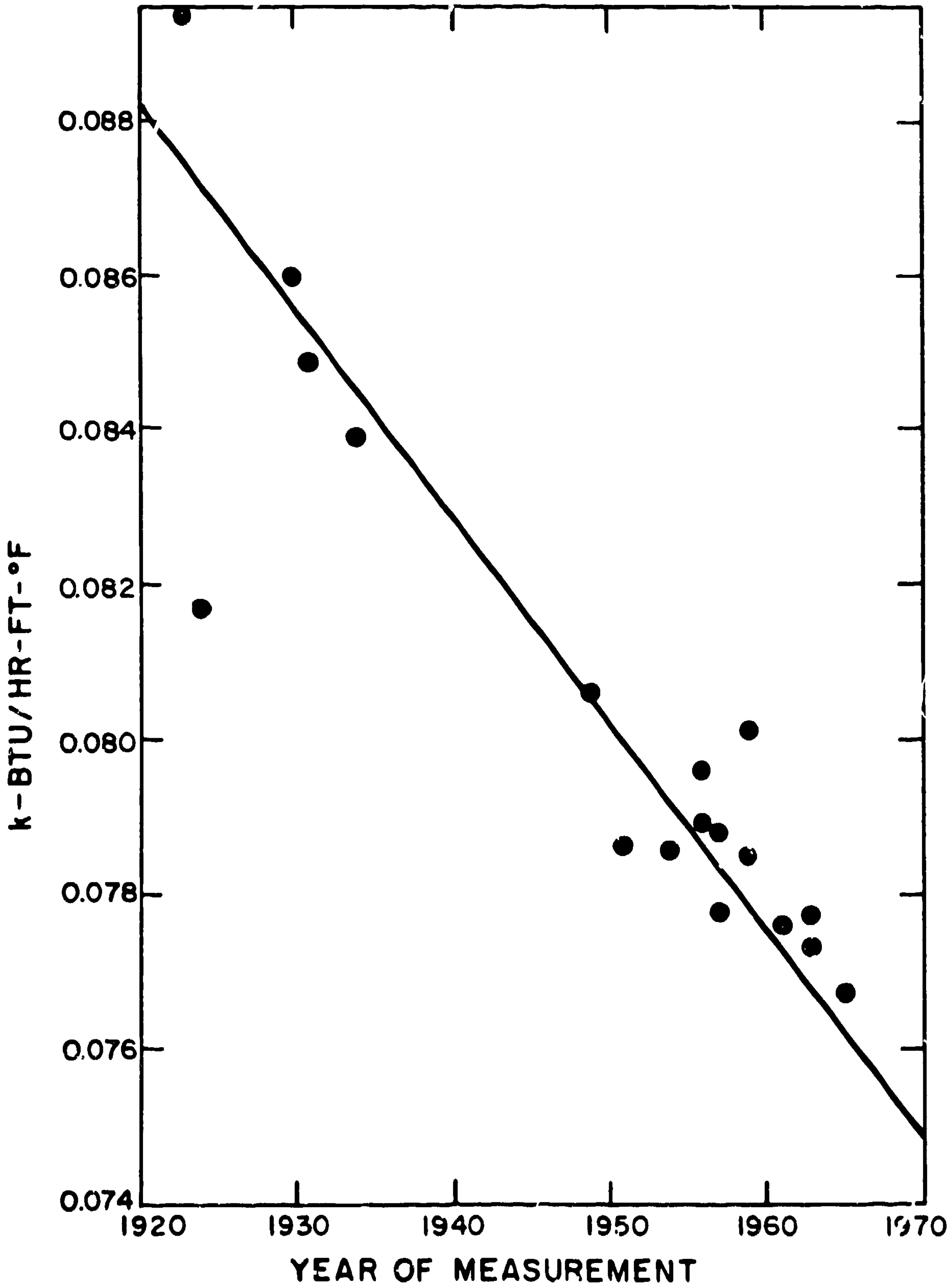

Fig. 4. Thermal Conductivity Measurements Since 1920 for Liquid Toluene at 20°C (Ref. 11)

3. RECOMMENDATIONS

The following recommendations are made for consideration by the readers.

I. There should be a continuous and well-supported effort by recognized experts in the field to understand the basic physical and chemical fundamentals behind variations in properties of matter. Basic research needs should be reviewed regularly to assure relevance. For example, Ref. 13 was prepared as a result of a survey of a small segment of the engineering community for basic research in fluid mechanics. The study of fundamental properties may become glamorous again.

II. Research and development programs should include funding and sufficient scheduling to permit new property measurements, as needed. To do so, early identification of basic research needs is required. Regular reviews and assessments can make this job easier. For example, Ref. 14 reports how computerization of chemical analysis data has been used successfully to identify several important trends in the occurrence of outgassing problems in aerospace programs.

III. It is incumbent upon every researcher reporting results in the literature to describe fully the measurement technique, accuracy obtained, environmental conditions at the time of measurement, and the history and condition of the sample. Critical evaluation of the data and meaningful comparison with other measurements can be done only when all are documented fully. Sometimes an analysis is no better than the laboratory making it. For example, different samples, different laboratories, and different techniques have caused a controversy about the existence of silica, as well as silicate, in the ash from Mt. St. Helens.[15] To standardize the type of sample being analyzed and to resolve the silica controversy, a round-robin testing program has been organized by the National Institute of Occupational Safety and Health.

IV. There are several important roles to be played by the scientific and professional societies. First, development of standards for reproducibility and accuracy of tests is an important task of organizations such as American Society for Testing Materials (ASTM), American National Standards Institute, and International Standards Organization. Regular topical symposia are used to focus on areas such as mechanical tests.[16] This should continue. Second, compilation and publication of property data are carried out by organizations such as American Institute of Chemical Engineers (Design Institute for Physical Properties Research), American Chemical Society and the American Institute of Physics (Journal of Physical and Chemical Reference Data), and ASTM (special technical publications). The existence of these resources should be made known to the scientific and engineering community.

V. Finally, efforts at periodic compilation and succinct publication of property data are to be supported, applauded, and extended, wherever possible. Particularly noteworthy are the publications "Mechanical Properties" and "Diffusion and Defect Data" by NBS. Most ambitious are the publications "Thermophysical Properties of Matter" by the Thermophysical Properties Research Center of CINDAS at Purdue University. This 20-year pioneering effort is a monumental accomplishment comprising 13 volumes with 43,604 data sets. Each point is fully referenced as to its original source. Critical evaluations of much data have been completed and more are under way. These evaluations will culminate in a "recommended" figure from among the various conflicting values reported (see Fig. 1).

In conclusion, we believe that while much has been accomplished, much remains to be done. Researchers of alternative energy sources must be in the forefront of those insisting that the understanding, collection, and critical compilation of information on properties of matter are carried out at a required level.

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